



NBS SPECIAL PUBLICATION 392

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Vibrationally Excited Hydrogen Halides:

A Bibliography on
Chemical Kinetics of Chemiexcitation
and Energy Transfer Processes
(1958 through 1973)

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Vibrationally Excited Hydrogen Halides: A Bibliography on Chemical Kinetics of Chemiexcitation and Energy Transfer Processes (1958 through 1973)

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This work was supported by the
NBS Office of Standard Reference Data
and
the Air Force Office of Scientific Research
1400 Wilson Blvd., Arlington, Va. 22209



U.S. DEPARTMENT OF COMMERCE, Frederick B. Dent, *Secretary*
NATIONAL BUREAU OF STANDARDS, Richard W. Roberts, *Director*

Issued April 1974

Supt. of Docs. No. C13.10:392

1. Chemical reaction, Rate of—Bibliography. 2. Hydrogen halides—Bibliography. 3. Energy transfer—Bibliography.

I. United States. National Bureau of Standards. Institute for Materials Research. Chemical Kinetics Information Center.

II. Title. III. Series: United States. National Bureau of Standards. Special Publication 392.

QC100.U57 No. 392 [Z5524.R5] 389'.08s 74-5358
[016.541'39]

National Bureau of Standards Special Publication 392

Nat. Bur. Stand. (U.S.), Spec. Publ. 392, 81 pages (Apr. 1974)

CODEN: XNBSAV

U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON: 1974

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402
(Order by SD Catalog No. C13.10:392). Price \$1.30

Foreword

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Further information on NSRDS and the publications which form the primary output of the program may be obtained by writing to the Office of Standard Reference Data, National Bureau of Standards, Washington, DC 20234.

David R. Lide, Jr., Chief
Office of Standard Reference Data

TABLE OF CONTENTS

| | |
|--|----|
| Introduction. | 1 |
| Guidelines for the user | 7 |
| Journal and report codes. | 11 |
| Part I. Hydrogen fluoride (HF, DF) | 15 |
| A. Formation of HF^\ddagger (DF^\ddagger) | 15 |
| 1. Bimolecular reactions (Abstraction lasers) | 15 |
| a. Abstraction of H (D) atom by F atom. | 15 |
| i. $\text{F} + \text{H}_2 \rightarrow \text{HF}^\ddagger + \text{H}$ | 15 |
| ii. $\text{F} + \text{HX} \rightarrow \text{HF}^\ddagger + \text{X}$ | 16 |
| iii. $\text{F} + \text{RH} \rightarrow \text{HF}^\ddagger + \text{R}$ | 17 |
| b. Abstraction of F atom by H (D) atom. | 17 |
| i. $\text{H} + \text{F}_2 \rightarrow \text{HF}^\ddagger + \text{F}$ | 17 |
| ii. $\text{H} + \text{FX} \rightarrow \text{HF}^\ddagger + \text{X}$ | 18 |
| iii. $\text{H} + \text{RF} \rightarrow \text{HF}^\ddagger + \text{R}$ | 18 |
| 2. Unimolecular reactions (Elimination lasers). | 18 |
| a. $\text{R}_1 + \text{R}_2 \rightarrow [\text{R}_1\text{R}_2]^* \rightarrow \text{HF}^\ddagger + \text{M}$ (Chemical activation).18 | |
| b. $\text{M}_1 + h\nu \rightarrow \text{HF}^\ddagger + \text{M}_2$ (Photochemical elimination) . .19 | |
| B. HF^\ddagger (DF^\ddagger) Energy transfer and quenching. | 19 |
| 1. HF^\ddagger (DF^\ddagger) Energy transfer. | 19 |
| a. $\text{HF}(v_i = 0) + \text{M}^\ddagger \rightarrow \text{HF}^\ddagger(v_j > 0) + \text{M}$ ($\text{M} \neq \text{HF}$) | |
| (Energy transferred to HF from M^\ddagger). | 19 |
| b. $\text{HF}^\ddagger(v_i = m) + \text{M} \rightarrow \text{HF}^\ddagger(v_j < m) + \text{M}^\ddagger$ ($v_j \geq 0$) | |
| (Energy transferred from HF^\ddagger to M). | 19 |
| c. $\text{HF}(v_i) + \text{HF}(v_j) \rightarrow \text{HF}(v_k) + \text{HF}(v_\ell)$ | |
| ($i + j = k + \ell$) (HF - HF Energy transfer) | 20 |
| 2. HF^\ddagger (DF^\ddagger) Quenching. | 21 |
| a. $\text{HF}^\ddagger(v_i = m) + \text{M} \rightarrow \text{HF}^\ddagger(v_j < m) + \text{M}$ ($v_j \geq 0$) | |
| (Collisional quenching) | 21 |
| b. $\text{HF}^\ddagger(v_i = m) + \text{HF} \rightarrow \text{HF}^\ddagger(v_j < m) + \text{HF}$ ($v_j \geq 0$) | |
| (HF - HF self-quenching). | 22 |
| c. $\text{HF}^\ddagger(v_i = m) + \text{M} \rightarrow \text{prod.}$ (Dissociative quenching) 22 | |
| i. $\text{HF}^\ddagger(v_i = m) + \text{M}_2 \rightarrow \text{HF}(v_j = 0) + \text{M} + \text{M}$ | 22 |
| ii. $\text{HF}^\ddagger(v_i = m) + \text{M} \rightarrow \text{H} + \text{F} + \text{M}$ | 23 |
| C. HF^\ddagger (DF^\ddagger) Theoretical papers | 23 |

| | |
|--|-----|
| Part II. Hydrogen chloride (HCl, DCl). | .24 |
| A. Formation of HCl^\ddagger (DCl^\ddagger) | .24 |
| 1. Bimolecular reactions (Abstraction lasers) | .24 |
| a. Abstraction of H (D) atom by Cl atom | .24 |
| i. $\text{Cl} + \text{H}_2 \rightarrow \text{HCl}^\ddagger + \text{H}$ | .24 |
| ii. $\text{Cl} + \text{HX} \rightarrow \text{HCl}^\ddagger + \text{X}$ | .24 |
| iii. $\text{Cl} + \text{RH} \rightarrow \text{HCl}^\ddagger + \text{R}$ | .25 |
| b. Abstraction of Cl atom by H (D) atom | .25 |
| i. $\text{H} + \text{Cl}_2 \rightarrow \text{HCl}^\ddagger + \text{Cl}$ | .25 |
| ii. $\text{H} + \text{ClX} \rightarrow \text{HCl}^\ddagger + \text{X}$ | .26 |
| iii. $\text{H} + \text{RCl} \rightarrow \text{HCl}^\ddagger + \text{R}$ | .26 |
| iv. $\text{H} + \text{HCl} \rightarrow \text{HCl}^\ddagger + \text{H}$ | .27 |
| 2. Unimolecular reactions (Elimination lasers) | .27 |
| a. $\text{R}_1 + \text{R}_2 \rightarrow [\text{R}_1\text{R}_2]^\ddagger \rightarrow \text{HCl}^\ddagger + \text{M}$ (Chemical activation) | .27 |
| b. $\text{M}_1 + h\nu \rightarrow \text{HCl}^\ddagger + \text{M}_2$ (Photochemical elimination) | .27 |
| B. HCl^\ddagger (DCl^\ddagger) Energy transfer and quenching. | .27 |
| 1. HCl^\ddagger (DCl^\ddagger) Energy transfer. | .27 |
| a. $\text{HCl}(\nu_i = 0) + \text{M}^\ddagger \rightarrow \text{HCl}^\ddagger(\nu_j > 0) + \text{M}$ ($\text{M} \neq \text{HCl}$) (Energy transferred to HCl from M^\ddagger) | .27 |
| b. $\text{HCl}^\ddagger(\nu_i = m) + \text{M} \rightarrow \text{HCl}^\ddagger(\nu_j < m) + \text{M}^\ddagger(\nu_j \geq 0)$ (Energy transferred from HCl^\ddagger to M) | .27 |
| c. $\text{HCl}(\nu_i) + \text{HCl}(\nu_j) \rightarrow \text{HCl}(\nu_k) + \text{HCl}(\nu_l)$ ($i + j = k + l$) (HCl - HCl Energy transfer) | .28 |
| 2. HCl^\ddagger (DCl^\ddagger) Quenching. | .28 |
| a. $\text{HCl}^\ddagger(\nu_i = m) + \text{M} \rightarrow \text{HCl}^\ddagger(\nu_j < m) + \text{M}$ ($\nu_j \geq 0$) (Collisional quenching) | .28 |
| b. $\text{HCl}^\ddagger(\nu_i = m) + \text{HCl} \rightarrow \text{HCl}^\ddagger(\nu_j < m) + \text{HCl}$ ($\nu_j \geq 0$) (HCl - HCl self-quenching) | .29 |
| c. $\text{HCl}^\ddagger(\nu_i = m) + \text{M}_2 \rightarrow \text{HCl}(\nu_j = 0) + \text{M} + \text{M}$ (Dissociative quenching) | .29 |
| C. HCl^\ddagger (DCl^\ddagger) Theoretical papers | .30 |

| | |
|--|----|
| Part III. Hydrogen bromide (HBr, DBr). | 31 |
| A. Formation of HBr^\ddagger (DBr^\ddagger) | 31 |
| 1. Bimolecular reactions (Abstraction lasers) | 31 |
| a. Abstraction of H (D) atom by Br atom | 31 |
| i. $\text{Br} + \text{H}_2 \rightarrow \text{HBr}^\ddagger + \text{H}$ | 31 |
| ii. $\text{Br} + \text{HX} \rightarrow \text{HBr}^\ddagger + \text{X}$ | 31 |
| iii. $\text{Br} + \text{RH} \rightarrow \text{HBr}^\ddagger + \text{R}$ | 31 |
| b. Abstraction of Br atom by H (D) atom | 31 |
| i. $\text{H} + \text{Br}_2 \rightarrow \text{HBr}^\ddagger + \text{Br}$ | 31 |
| ii. $\text{H} + \text{BrX} \rightarrow \text{HBr}^\ddagger + \text{X}$ | 32 |
| B. HBr^\ddagger (DBr^\ddagger) Energy transfer and quenching. | 32 |
| 1. HBr^\ddagger (DBr^\ddagger) Energy transfer. | 32 |
| a. $\text{HBr}(v_i = 0) + \text{M}^\ddagger \rightarrow \text{HBr}^\ddagger(v_j > 0) + \text{M}$ ($\text{M} \neq \text{HBr}$) (Energy transferred to HBr from M^\ddagger) | 32 |
| b. $\text{HBr}^\ddagger(v_i = m) + \text{M} \rightarrow \text{HBr}^\ddagger(v_j < m) + \text{M}^\ddagger$ ($v_j \geq 0$) (Energy transferred from HBr^\ddagger to M) | 32 |
| c. $\text{HBr}(v_i) + \text{HBr}(v_j) \rightarrow \text{HBr}(v_k) + \text{HBr}(v_l)$ ($i + j = k + l$) (HBr - HBr Energy transfer) | 32 |
| 2. HBr^\ddagger (DBr^\ddagger) Quenching. | 32 |
| a. $\text{HBr}^\ddagger(v_i = m) + \text{M} \rightarrow \text{HBr}^\ddagger(v_j < m) + \text{M}$ ($v_j \geq 0$) (Collisional quenching) | 32 |
| b. $\text{HBr}^\ddagger(v_i = m) + \text{HBr} \rightarrow \text{HBr}^\ddagger(v_j < m) + \text{HBr}$ ($v_j \geq 0$) (HBr - HBr self-quenching). | 33 |
| C. HBr^\ddagger (DBr^\ddagger) Theoretical papers. | 33 |

| | |
|--|----|
| Part IV. Hydrogen iodide (HI, DI) | 34 |
| A. Formation of HI^\ddagger (DI^\ddagger) | 34 |
| 1. Bimolecular reactions (Abstraction lasers) | 34 |
| a. Abstraction of H (D) atom by I atom. | 34 |
| i. $\text{I} + \text{H}_2 \rightarrow \text{HI}^\ddagger + \text{H}$ | 34 |
| ii. $\text{I} + \text{HX} \rightarrow \text{HI}^\ddagger + \text{X}$ | 34 |
| iii. $\text{I} + \text{RH} \rightarrow \text{HI}^\ddagger + \text{R}$ | 34 |
| b. Abstraction of I atom by H (D) atom. | 34 |
| i. $\text{H} + \text{I}_2 \rightarrow \text{HI}^\ddagger + \text{I}$ | 34 |
| ii. $\text{H} + \text{IX} \rightarrow \text{HI}^\ddagger + \text{X}$ | 34 |
| B. HI^\ddagger (DI^\ddagger) Energy transfer and quenching. | 34 |
| 1. HI^\ddagger (DI^\ddagger) Energy transfer. | 34 |
| a. $\text{HI}(v_i = 0) + \text{M}^\ddagger \rightarrow \text{HI}^\ddagger(v_j > 0) + \text{M}$ ($\text{M} \neq \text{HI}$) | |
| (Energy transferred to HI from M^\ddagger) | 34 |
| b. $\text{HI}^\ddagger(v_i = m) + \text{M} \rightarrow \text{HI}^\ddagger(v_j < m) + \text{M}^\ddagger$ ($v_j \geq 0$) | |
| (Energy transferred from HI^\ddagger to M) | 35 |
| c. $\text{HI}(v_i) + \text{HI}(v_j) \rightarrow \text{HI}(v_k) + \text{HI}(v_l)$ | |
| ($i + j = k + l$) (HI - HI Energy transfer) | 35 |
| 2. HI^\ddagger (DI^\ddagger) Quenching. | 35 |
| a. $\text{HI}^\ddagger(v_i = m) + \text{M} \rightarrow \text{HI}^\ddagger(v_j < m) + \text{M}$ ($v_j \geq 0$) | |
| (Collisional quenching) | 35 |
| b. $\text{HI}^\ddagger(v_i = m) + \text{HI} \rightarrow \text{HI}^\ddagger(v_j < m) + \text{HI}$ ($v_j \geq 0$) | |
| (HI - HI self-quenching) | 35 |
| C. HI^\ddagger (DI^\ddagger) Theoretical papers | 35 |
| Part V. Reviews and Bibliographies | 36 |
| Part VI. References | 37 |

A Bibliography on Chemical Kinetics of Chemi-excitation
and Energy Transfer Processes*

Francis Westley

A bibliography, a reaction oriented list of references, is provided for published papers and reports containing rate data for reactions of halogen atoms with hydrogen-containing compounds, or of H (D, or T) atoms with halogen-containing compounds to form vibrationally chemiexcited hydrogen halides. The reactions for vibroexcitation of hydrogen halides through unimolecular or photochemical elimination, as well as the processes for vibrational energy transfer between hydrogen halides and various second bodies are also included. In addition, four lists of theoretical papers and a list of critical reviews and bibliographies are provided. Over 300 papers covering 50 types of reactions are listed. The period covered extends from 1958 through 1973.

Key words: Bibliography; chemical kinetics; chemiexcitation; gas phase; halogens; hydrogen; hydrogen halides; laser; quenching; vibrational energy transfer.

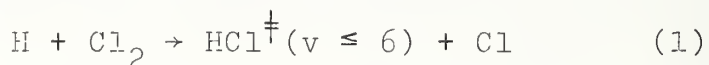
Introduction

The bibliography lists papers and reports on the gas phase reaction kinetics of two types of chemical processes: a) formation of vibrationally excited hydrogen halides through abstraction or elimination and b) vibrational energy transfer - including quenching - between hydrogen halides and various second bodies.

*This publication is an activity of the Chemical Kinetics Information Center, National Bureau of Standards. The work was supported by the Office of Standard Reference Data, National Bureau of Standards and the Air Force Office of Scientific Research as part of a program to provide information and data on rates of chemical reactions.

The articles have been selected from the files of the Chemical Kinetics Information Center. The criterion for inclusion of an article is that it must contain some new information on the reaction. That is, simple quotations of the results of others and ad hoc guesses have been excluded. There are gray areas, such as the statement of a rate calculated from that of the reverse reaction and the equilibrium constant, or information such as: suggestion of a new mechanism, or a theoretical calculation, or a new theoretical approach derived from kinetic experiments. If the information seemed to be important the reference was included.

The two above mentioned types of reactions (formation of vibrationally excited hydrogen halides and transfer of vibrational energy between hydrogen halides and other bodies) are essential in a fairly new branch of quantum electronics: the chemical laser. Light amplification by stimulated emission of radiation (in short: laser) is a fairly recent development in science dealing with the generation of coherent radiation in the infrared and visible regions of the spectrum. The chemical lasers are based on the new principle of obtaining energy - in the form of coherent radiation - from chemical reactions: the principle of "chemical pumping". In other words, chemical interaction between two gaseous molecules results in the pumping of electronic, vibrational, or rotational energy into the newly formed bond of one to the reaction products. The new bond "stores" for a short time an amount of energy available for other uses. Such a reaction, which is only the first elementary step in the more complex lasing process, is called in short "chemiexcitation". The first observation of an infrared emission from the reaction of atomic hydrogen with molecular chlorine, was reported in 1958 by Cashion and Polanyi^{1,2}. They attributed this emission to the vibrationally excited hydrogen chloride, which was one of the products of the reaction:



In 1961, Polanyi suggested the construction of a HCl laser, dependent on vibrational excitation, which would operate in the infrared region⁸. Polanyi and coworkers have continued their pioneering work in the field of chemical lasers, by following a double path: experimental [infrared spectroscopy^{3,4,5}], energy distribution among reaction products^{6,13,14,17,18,29,21,22,23}] and theoretical [energy distribution^{7,9,10,12,15,19,23}], potential energy surface^{11,12,23}], trajectories^{12,15,23}], chemical kinetics¹⁶].

However, the first description of an operational HCl pulsed chemical laser was published in 1965 by Kasper and Pimentel²⁴⁾. In the following years the research on chemical lasers has been continually expanding. A list of the universities and industrial research laboratories, as well as of their scientists carrying out research in chemical lasers can be found in the introduction of a bibliography published in 1972 by the U.S. Atomic Energy Commission [Chemical Lasers: An Overview of the Literature, (1960 - 1971)²⁵⁾].

Since 1965, many chemiexcited molecules have been found suitable in the operation of chemical lasers. However, the hydrogen halides are the most used molecules for that purpose. To date, the highest energy level of a chemiexcited hydrogen halide molecule is vibrational. The search of the literature failed to show the existence of a laser based on an electronically excited hydrogen halide molecule. For these reasons, this bibliography is confined only to two types of reactions involving hydrogen halides: a) vibrational chemiexcitation and b) vibrational energy transfer. No attempt was made to cover the literature dealing with the operation of hydrogen halide lasers. The reader interested in operation of chemical lasers should consult the "Comprehensive Literature Survey of Chemical Lasers" by Arnold and Rojeska²⁶⁾ or the above mentioned bibliography of Dobratz²⁵⁾, as well as other reviews and bibliographies listed in part V of this work.

This bibliography is not the result of the effort of a single person, but of the whole staff of Chemical Kinetics Information Center. My thanks to all of them.

In particular, I wish to thank Dr. David Garvin, Director of the Center, and Dr. Robert Hampson for their more than helpful suggestions and constant guidance; Mr. James G. Koch, Supervisor, for tracking down and obtaining papers and reports, otherwise very difficult to obtain; Mrs. Ann C. Robertson, Mrs. Geraldine Zumwalt and Miss Darlene Connelly, for typing a difficult manuscript with particular care.

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Arrangement of the report. This bibliography is in six parts:

- Part I. Hydrogen fluoride (HF^\ddagger , or DF^\ddagger)
Part II. Hydrogen chloride (HCl^\ddagger , or DCl^\ddagger)
Part III. Hydrogen bromide (HBr^\ddagger , or DBr^\ddagger)
Part IV. Hydrogen iodide (HI^\ddagger , or DI^\ddagger)
Part V. Reviews and Bibliographies (Critical reviews, or surveys and general bibliographies dealing with the reactions listed in parts I to IV).
Part VI. The combined bibliography for Parts I to V arranged alphabetically by authors. The complete reference citation for each article mentioned is given here. Occasionally explanatory notes are appended. These establish the "bibliography chain" for closely related papers by the same authors.

Parts I to IV are arranged in the order of their importance: Hydrogen fluoride (Part I) is the most intensively studied chemical laser, while hydrogen iodide (Part IV) is the least studied.

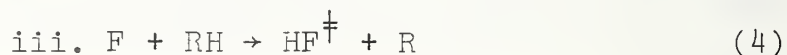
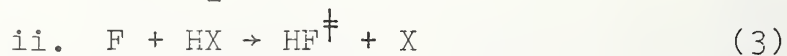
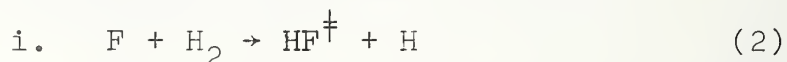
Ordering of chemical reactions. The purpose of this work is to provide the chemical kineticist with a useful list of articles and papers dealing with the vibrationally excited hydrogen halides. For that reason, the arrangement of the bibliography is reaction oriented: parts I to IV are each divided into three large sections:

- Section A. Formation of HX^\ddagger ($\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$)
Section B. HX^\ddagger Energy Transfer and Quenching
Section C. HX^\ddagger Theoretical Papers

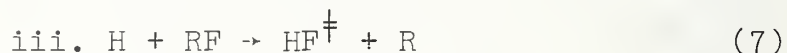
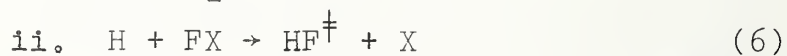
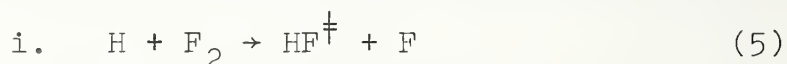
The titles of Sections A and B define very broad categories of reactions. Section C includes only theoretical papers, very closely related to the kinetics of vibrationally excited hydrogen halides. Section A does not include formation of HX^\ddagger by energy transfer. This type of reaction may be found in Section B, under 1.a. Each of the Sections A and B is divided into smaller categories of reactions and so on, as indicated in the table of contents.

Display of Chemical Reactions and Formulae. With the exception of subgroups A.1.a and A.1.b, all the other subgroups define a type of chemical reaction. Subgroups A.1.a and A.1.b are each further divided into three types of reactions. For instance, in part I (Hydrogen fluoride) these types are:

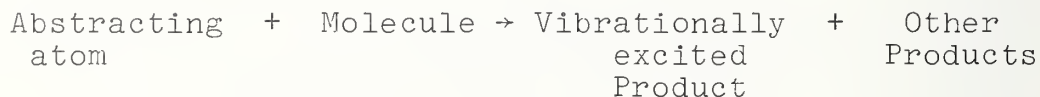
A.1.a. Abstraction of H atom by F atom.



A.1.b. Abstraction of F atom by H atom.

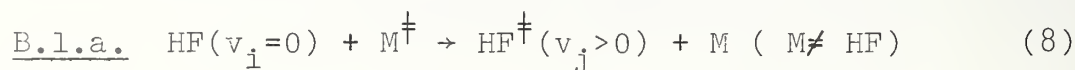


Throughout the work these different types of reactions are displayed according to a scheme trying to emphasize the direction and nature of the chemical process, rather than to follow a mere alphabetical order. So, the above listed reactions (2) to (7) are all written according to the invariable pattern:

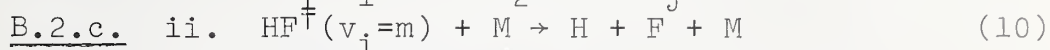
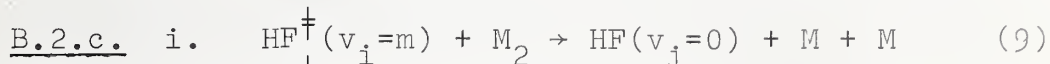


In reactions (4) and (7), the terms RH and RF denote in general a hydrogen containing - and, respectively, a halogen containing - organic molecule. However, in some instances, a reference listed under the headings A.1.a.iii. or A.1.b.iii. (Reactions (4) and (7)), might deal with a hydrogen - or halogen - containing inorganic molecule.

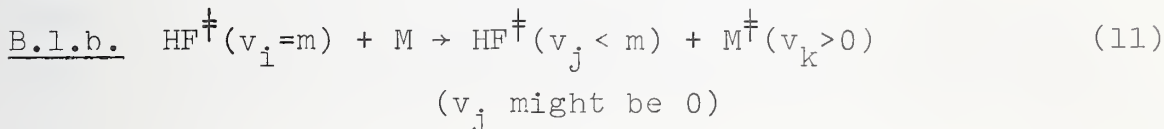
The general "third body", whether excited or in ground state, is always last:



In general, the first term at the right side of a reaction indicates a vibrationally excited product. The only exception is the reaction type B.2.c (Dissociative quenching).



Excited states of reactants and products. This bibliography deals exclusively with vibrationally excited hydrogen halides. The sign used to indicate the vibronic state of a molecule is the double dagger superscript. If the double dagger appears inside a bracket, it indicates that the molecule might be in its ground state (zero vibrational level):



Only in one instance an asterisk is used to indicate the formation of an intermediate activated complex, which subsequently is dissociated into a vibrationally excited hydrogen halide molecule and another product:



Reactions of the type B.1.c. are expressed by a generalized chemical equation including all the $\text{HX} - \text{HX}$ vibrational energy transfer processes. The multiplicity of vibrational levels (some authors consider 8 vibrational levels in the same paper) would have made it very difficult to arrange this bibliography according to all the possible $\text{HX} - \text{HX}$ vibronic interactions. Although, in this type of process, four different vibronic levels coexist, the double dagger superscript is entirely omitted and the different vibronic levels are indicated in a bracket following each HX molecule. The reason for omitting the dagger symbol is that only one of the four vibronic levels (v_i, v_j, v_k, v_l) may be zero, provided that the condition $i + j = k + l$ is satisfied. (If two, or three of these vibronic levels are zero, then the process becomes a simple quenching, or excitation one.). For the case of the $\text{HF} - \text{HF}$ vibrational energy transfer, the B.1.c. process is indicated as follows:



(only one of four levels v_i, v_j, v_k, v_l may be zero)

Reference Citations.

The references under each reaction list the author(s) and the sources, in the following form:

| Author(s) | Source-Year-Volume-Page | Number of Author(s) |
|-----------------|-------------------------|---------------------|
| Airey, J. R. | IJCKBO-1970-2-65 | 1 |
| Airey and Fried | CHPLBC-1971-8-23 | 2 |
| Airey, et al. | JCPA6-1964-41-3255 | 3 or more |

Variations from this format (which we will call "short reference") are usually in the direction of more explicit specification. These variations are never made in the first two fields, source and year. They are fixed and always present.

The sources are indicated by their ASTM CODEN abbreviations^{*}). A guide to these codes follows. As listed in this guide, the codes include an additional sixth cipher, which is a "check character"^{**}). A code prefixed with an asterisk is a code not in the ASTM CODEN set. These are codes we have assigned for reports from industrial laboratories, research institutes and universities. When the CODEN system adopts appropriate codes they will be replaced. The present, temporary codes usually end with Z or U.

^{*}) Blumental, J. G., Karaman, M., Editors, "CODEN FOR PERIODICAL TITLES" (Including Non-Periodical Titles and Deleted Coden), Vol. I and II, ASTM Data Series DS 23B, Third Edition, (1970); Padusis, M., Editor, First Supplement to Third Edition, DS 23B-S1 (05-023021-42, 1972). (American Society for Testing and Materials, 1916 Race St., Philadelphia, Pa. 19103)

^{**}) The final sixth character in the journal code is a "check character". This is not shown in the listings in ASTM DS 23B and DS 23B-S1, but the calculation is explained in the introductions to them. See also "Subroutine for the Calculation of CODEN Check Characters, D. Garvin, National Bureau of Standards, Tech. Note 738 (Sept. 1972)

JOURNAL AND REPORT CODES

| | |
|---------|--|
| ACHRAY | ACCOUNTS OF CHEMICAL RESEARCH (Washington) |
| ACIEAY | ANGEWANDTE CHEMIE (International Edition in English) |
| ACSRAL | AMERICAN CHEMICAL SOCIETY, ABSTRACT OF PAPERS |
| ADCPAA | ADVANCES IN CHEMICAL PHYSICS (New York) |
| AOPAI | APPLIED OPTICS (Washington) |
| APOSAR | APPLIED OPTICS, SUPPLEMENT (Washington) |
| APPLAB | APPLIED PHYSICS LETTERS (New York) |
| ARPLAP | ANNUAL REVIEW OF PHYSICAL CHEMISTRY |
| *ASTSZU | THE AEROSPACE CORPORATION |
| BBPCAX | BERICHTE DER BUNSENGESELLSCHAFT FUER PHYSIKALISCHE CHEMIE (Germany) |
| BOOKA7 | BOOK |
| CBFMAO | COMBUSTION AND FLAME |
| CCHKAZ | COMPREHENSIVE CHEMICAL KINETICS (Amsterdam) |
| CHDBAN | COMPTES RENDUS HEBDOMADAIRES DES SEANCES DE L'ACADEMIE DES SCIENCES, SERIE B. SCIENCES PHYSIQUES (Paris) |
| CHMBAY | CHEMISTRY IN BRITAIN (London) |
| CHPLBC | CHEMICAL PHYSICS LETTERS (Amsterdam) |
| CITEAH | CHEMIE-INGENIEUR-TECHNIK (Germany) |
| CJCHAG | CANADIAN JOURNAL OF CHEMISTRY |
| CSSPAD | CHEMICAL SOCIETY, SPECIAL PUBLICATION (London) |
| DABBBA | DISSERTATION ABSTRACTS INTERNATIONAL, B. THE SCIENCES AND ENGINEERING |
| DABSA9 | DISSERTATION ABSTRACTS PART B. SCIENCES AND ENGINEERING |
| DAKEAT | DANSK KEMI (Copenhagen) |
| DFSOAW | DISCUSSIONS OF FARADAY SOCIETY |
| DIASA9 | DISSERTATION ABSTRACTS |
| DKPCAG | DOKLADY PHYSICAL CHEMISTRY, PROCEEDINGS OF THE ACADEMY OF SCIENCES OF THE USSR (New York) |
| HIECAP | HIGH ENERGY CHEMISTRY (New York) |
| IEJQA7 | IEEE JOURNAL OF QUANTUM ELECTRONICS (New York) |
| IJCKBO | INTERNATIONAL JOURNAL OF CHEMICAL KINETICS (New York) |

| | |
|--------|--|
| JAPIAU | JOURNAL OF APPLIED PHYSICS (New York) |
| JASMAN | JOURNAL OF THE ACOUSTICAL SOCIETY OF AMERICA |
| JCFTAR | JOURNAL OF CHEMICAL SOCIETY, FARADAY TRANSACTIONS I (London) |
| JCFTBS | JOURNAL OF CHEMICAL SOCIETY, FARADAY TRANSACTIONS II (London) |
| JCPQAY | JOURNAL DE CHIMIE PHYSIQUE |
| JCPSA6 | JOURNAL OF CHEMICAL PHYSICS |
| JCSOA9 | JOURNAL OF THE CHEMICAL SOCIETY (London) |
| JPCHAX | JOURNAL OF PHYSICAL CHEMISTRY |
| JQSRAE | JOURNAL OF QUANTITATIVE SPECTROSCOPY AND RADIATIVE TRANSFER |
| JTPLA2 | JETP LETTERS, SOVIET PHYSICS (New York) |
| KICAA8 | KINETICS AND CATALYSIS |
| LSRVAN | LASER FOCUS |
| MOPHAM | MOLECULAR PHYSICS (London) |
| NATUAS | NATURE (London) |
| PACHAS | PURE AND APPLIED CHEMISTRY (London) |
| PRKNAZ | PROGRESS IN REACTION KINETICS |
| PRLAAZ | PROCEEDINGS OF ROYAL SOCIETY, SERIES A. MATHEMATICAL AND PHYSICAL SCIENCES (London) |
| PRLTAO | PHYSICAL REVIEW LETTERS (New York) |
| PYLAAG | PHYSICS LETTERS, SECTION A (Amsterdam) |
| QRCSAL | QUARTERLY REVIEW OF THE CHEMICAL SOCIETY (London) |
| RJPCAR | RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY |
| SCAMAC | SCIENTIFIC AMERICAN (New York) |
| SCIEAS | SCIENCE (Washington) |
| SPHJAR | SOVIET PHYSICS JETP (New York) |
| SPUSBI | SOVIET PHYSICS - USPEKHI (New York) |
| SYMCAQ | SYMPOSIUM ON COMBUSTION |
| TFSOA4 | TRANSACTIONS OF THE FARADAY SOCIETY |
| UCRLAE | UNIVERSITY OF CALIFORNIA, LAWRENCE RADIATION LABORATORY, REPORTS |
| XADRCH | UNITED STATES DEPARTMENT OF COMMERCE, NATIONAL TECHNICAL INFORMATION SERVICE |
| XCCIAV | UNITED STATES DEPARTMENT OF COMMERCE, CLEARINGHOUSE FOR SCIENTIFIC AND TECHNICAL INFORMATION |

XERLAR U.S. ATOMIC ENERGY COMMISSION, UNIVERSITY OF
CALIFORNIA, RADIATION LABORATORY

ZEPCAC ZEITSCHRIFT FÜR PHYSIKALISCHE CHEMIE, STOECHIO-
METRIE UND VERWANDTSCHAFTSLIHE

ZPCBAL ZEITSCHRIFT FÜR PHYSIKALISCHE CHEMIE, ABTEILUNG B:
CHEMIE DER ELEMENTARPROZESSE, AUFBAU DER MATERIE

26BMAD MTP(MEDICAL AND TECHNICAL PUBLISHING COMPANY)
INTERNATIONAL REVIEW OF SCIENCE: PHYSICAL CHEMISTRY,
SERIES ONE 1972-1973

Abbreviations

The abbreviations listed below, are used in parts I through IV of this bibliography.

| | |
|----------------|------------------------------|
| (calc.) | = (calculation) |
| (cr. sect.) | = (cross section) |
| (d.r.) | = (detailed rates) |
| (mech.) | = (mechanism) |
| (model.) | = (modelling) |
| (pop. distr.) | = (population distribution) |
| (pot. surf.) | = (potential energy surface) |
| (r.p.) | = (related paper) |
| (rev.) | = (review) |
| (traj.) | = (trajectories) |
| (trans. prob.) | = (transition probability) |

They are appended inside brackets at the end of the short references. In general, a short reference without appended abbreviations indicates a work including rate constants while a reference followed by appended abbreviations may or may not include rate constants.

The abbreviation r.p. (related paper) indicates a paper which cannot fit in any of the above listed categories. For instance, a work dealing with laser operation will be followed by (r.p.) if it is considered of interest. However, a number of papers with rate constants are included in the r.p. category. For instance, under the heading: $\text{Cl} + \text{H}_2 \rightarrow \text{HCl}^\dagger + \text{H}$ a number of papers giving rate constants for the overall reaction $\text{Cl} + \text{H}_2 \rightarrow \text{HCl} + \text{H}$ are included. In this reaction, the product HCl indicates all molecules of hydrogen chloride whether in the ground state or in an excited state. Such a paper is therefore a very closely related paper.

Part I. Hydrogen fluoride (HF, DF)

A. Formation of HF^\ddagger (DF^\ddagger)

1. Bimolecular Reactions (Abstraction Lasers)

a. Abstraction of H(D) Atom by F Atom

i. $\text{F} + \text{H}_2 \rightarrow \text{HF}^\ddagger + \text{H}$

| | |
|-------------------------|---|
| Airey, J. R. | IJCKBO-1970-2-65 |
| Anlauf, et al. | JCPSA6-1970-53-4091 (calc., pop. distr.) |
| Basov, et al. | JTPLA2-1969-9-375 (r. p.) |
| Beattie, et al. | IEJQA7-1973-9-202 (r.p.) |
| Ben-Shaul, et al. | JCPSA6-1972-57-5427 (calc., pop. distr.) |
| Ben-Shaul, et al. | CHPLBC-1972-15-160 (pop. distr.) |
| Berry, M. J. | ACSRAL-1973-166-Phys. 98 |
| Brokaw, R. S. | JPCHAX-1965-69-2808 (r. p.) |
| Burmasov, et al. | JTPLA2-1969-10-28 (r. p.) |
| Chang and Setser | JCPSA6-1973-58-2298 (pop. distr.) |
| Chester and Hess | IEJQA7-1972-8-1 (rev.) |
| Clyne, et al. | CJCHAG-1973-51-3596 (r. p.) |
| Cohen, N. | XADRCA-1972-AD 763715 |
| Cool, et al. | APPLAB-1969-15-318 (r. p.) |
| Cool, et al. | JAPIAU-1970-41-4038 |
| Coombe and Pimentel | IEJQA7-1973-9-192 |
| Coombe and Pimentel | JCPSA6-1973-59-251 |
| Coombe and Pimentel | JCPSA6-1973-59-1535 |
| Deutsch, T. F. | APPLAB-1967-10-234 (r. p.) |
| Deutsch, T. F. | APPLAB-1967-11-18 (r. p.) |
| Dodonov, et al. | DKPCAG-1971-198-440 |
| Dolgov-Savel'ev, et al. | SPHJAR-1970-31-643 |
| Duewer and Setser | JCPSA6-1973-58-2310 (pop. distr.) |
| Dolgov-Savel'ev, et al. | SPHJAR-1972-34-34 |
| Emanuel, et al. | XADRCA-1972-AD 746685 (rev.) |
| Fettis and Knox | PRKNAZ-1964-2-2 (r. p.) |
| Green and Lin | JCPSA6-1971-74-3222 (calc.) |
| Gregg, et al. | CHPLBC-1971-8-609 (r. p.) |
| Gross, R. W. F. | JCPSA6-1969-50-1889 (r. p.) |
| Gross, et al. | JCPSA6-1968-48-3821 (r. p.) |
| Gross, et al. | JCPSA6-1969-51-1250 (r. p.) |
| Gross, et al. | IEJQA7-1970-6-168 (r. p.) |
| Hess, L. D. | IEJQA7-1973-9-201 (r. p.) |
| Hess, L. D. | JAPIAU-1972-43-1157 (r. p.) |
| Hess, L. D. | JCPSA6-1971-55-2466 |
| Homann, et al. | BBPCAX-1970-74-585 (r. p.) |
| Jaffe, et al. | JCPSA6-1973-59-1128 (calc., pot. surf., traj.) |
| Jensen and Rice | CHPLBC-1970-7-627 (r. p.) |
| Jensen and Rice | CHPLBC-1971-8-214 (r. p.) |
| Jonathan, et al. | MOPHAM-1971-20-93 |
| Jonathan, et al. | APOPAT-1971-10-1821 |
| Kapralova and Chaikin | CBFMAO-1969-13-557 (r. p.) |
| Kapralova, et al. | KICAA8-1970-11-669 (r. p.) |

Jonathan, et al.
Jonathan, et al.
Kirsch and Polanyi
Kompa and Wanner

CHPLBC-1970-7-257
APOPAT-1971-10-1821 (calc.)
JCPSA6-1972-57-4498 (calc.)
CHPLBC-1972-12-560

iii. $F + RH \rightarrow HF^{\ddagger} + R$

Berry, M. J.
Brus and Lin
Chang and Setser
Chang, et al.
Chang, et al.
Clyne, et al.
Creighton, et al.
Duewer and Setser
Fettis, et al.
Green and Lin
Gregg, et al.
Jacobson and Kimbell
Jacobson and Kimbell
Johnson, et al.

IEJQA7-1973-9-199 (r. p.)
JPCHAX-1971-75-2546
JCPSA6-1973-58-2298 (pop. distr.)
JPCHAX-1971-75-2070
CHPLBC-1971-9-587
CJCHAG-1973-51-3596 (r. p.)
IEJQA7-1973-9-200
JCPSA6-1973-58-2310 (pop. distr.)
JCPSA6-1960-1064 (r. p.)
JCPSA6-1971-54-3222
CHPLBC-1971-8-609
CHPLBC-1971-8-309 (r. p.)
JAPIAU-1971-42-3402 (r. p.)
JPCHAX-1973-77-2499 (calc., pop. distr.,
pot. surf., traj.)

Jonathan, et al.
Jonathan, et al.
Kapralova, et al.
Kim and Setser
Kim and Setser
Kompa, et al.
Kompa and Wanner
Krogh and Pimentel
Lin and Green
Mercer and Pritchard
Molina and Pimentel
Padrick and Pimentel
Parker and Pimentel
Parker and Pimentel
Parker and Pimentel
Pimentel, G. C.
Pimentel, G. C.
Suchard and Pimentel
Vedeneev, et al.

MOPHAM-1971-20-93
APOPAT-1971-10-1821
KICAA8-1970-11-669 (r. p.)
ACSRAL-1973-166-Phys. 99
JPCHAX-1973-77-2493 (pop. distr.)
CHPLBC-1969-3-210 (r. p.)
CHPLBC-1972-12-560
JCPSA6-1972-56-969
JCPSA6-1970-53-3383
JPCHAX-1959-63-1468 (r. p.)
IEJQA7-1973-9-64
APPLAB-1972-20-167
IEJQA7-1970-6-175
JCPSA6-1968-48-5273 (r. p.)
JCPSA6-1971-55-857
DAKEAT-1969-50-1 (rev.)
IEJQA7-1970-6-174 (rev.)
APPLAB-1971-18-530
KICAA8-1963-4-278 (r. p.)

b. Abstraction of F Atom by H(D) Atom

i. $H + F_2 \rightarrow HF^{\ddagger} + F$

Airey, J. R.
Albright, et al.
Basov, et al.
Burmastov, et al.
Cohen, N.
Cool, et al.
Cool, et al.
Dodonov, et al.

IJCKBO-1970-2-65
JCPSA6-1969-50-3632
JTPLA2-1969-9-375 (r. p.)
JTPLA2-1969-10-28 (r. p.)
XADRCA-1972-AD 763715
APPLAB-1969-15-318 (r. p.)
JAPIAU-1970-41-4038
KICAA8-1970-11-677

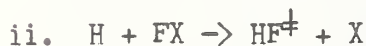
Emanuel, et al.
Hess, L. D.
Jonathan, et al.
Jonathan, et al.
Jonathan, et al.

XADRCA-1972-AD 746685 (rev.)
JCPSA6-1971-55-2466
JCPSA6-1970-53-4396 (r. p.)
APOPAI-1971-10-1821 (calc.)
MOPHAM-1972-24-1143 (calc., pot. surf.,
traj.)

Kapralova and Chaikin
Kerber, et al.
Kerber and Whittier
Kompa, K. L.
Levy and Copeland
Levy and Copeland
Levy and Copeland
Mayer, et al.
O'Neil, et al.
Polanyi and Sloan
Semenov and Shilov
Slootmaekers and Van Tiggelen
Suchard, et al.
Suchard, et al.
Suchard, et al.
Tal'roze, et al.
Vedeneev, et al.
Vedeneev, et al.
Wilkins, R. L.

CBFMAO-1969-13-557 (mech.)
IIEJQA7-1973-9-94 (rev.)
*ASTSZx-1970-TOR-0059(6753-10)-1
CITEAH-1970-42-573 (rev.)
JPCHAX-1963-67-2156 (mech.)
JPCHAX-1965-69-408 (r. p.)
JPCHAX-1968-72-3168 (r. p.)
SYMCAQ-1967-11-837 (r. p.)
JCPSA6-1973-58-1126 (calc., pot. surf.)
JCPSA6-1972-57-4988 (calc., d.r.)
KICAA8-1964-6-1 (mech.)
BSCBAG-1958-67-135 (r. p.)
APPLAB-1971-19-411 (r. p.)
JCPSA6-1972-57-5065
XADRCA-1973-AD 763716
KICAA8-1970-11-233
KICAA8-1963-4-278 (r. p.)
RJPCAR-1969-43-713
JCPSA6-1973-58-2326 (calc., d.r., pot. surf.,
traj.)
XADRCA-1971-AD 725031 (calc.)
APPLAB-1972-20-64 (r. p.)

Wilkins, R. L.
Wilson and Stephenson



Krogh and Pimentel
Mayer, et al.
Pimentel, G. C.

JCPSA6-1972-56-969
SYMCAQ-1967-11-837 (r. p.)
JCPSA6-1973-58-1270 (r. p.)



Cross, J. B.
Gensel, et al.
Herbelin and Cohen
Krogh and Pimentel
Perona, M. J.
Pimentel, G. C.
Rabideau, S. W.

JCPSA6-1973-59-966 (r. p.)
CHPLBC-1970-5-179 (r. p.)
CHPLBC-1973-20-605 (r. p.)
JCPSA6-1972-56-969
JCPSA6-1971-54-4024
JCPSA6-1973-58-1270 (r. p.)
JCPSA6-1973-59-1533

2. Unimolecular Reactions (elimination lasers)



Berry, M. J.
Berry and Pimentel
Berry and Pimentel

DABBBA-1971-31-7210
IEJQA7-1970-6-176
JCPSAC-1968-49-5190

| | |
|-------------------------------|-----------------------------|
| Brus and Lin | JPCHAX-1971-75-2546 |
| Clough, et al. | CJCHAG-1970-48-2919 |
| Cuellar-Ferreira and Pimentel | IEJQA7-1973-9-201 |
| Gordon and Lin | ACSRAL-1973-166-Phys. 137 |
| Lin, M. C. | IEJQA7-1973-9-200 (r. p.) |
| Lin, M. C. | JPCHAX-1971-75-3642 |
| Padrick and Pimentel | APPLAB-1972-20-167 |
| Padrick and Pimentel | JCPSA6-1971-54-720 |
| Pimentel, G. C. | IEJQA7-1970-6-174 (rev.) |
| Roebber and Pimentel | IEJQA7-1973-9-201 (r. p.) |
| Ross and Shaw | JPCHAX-1971-75-1170 (r. p.) |

b. $M_1 + h\nu \rightarrow HF^{\ddagger} + M_2$ (photochemical elimination)

| | |
|--------------------|-----------------------------|
| Berry, M. J. | DABBBA-1971-31-7210 |
| Berry and Pimentel | IEJQA7-1970-6-176 |
| Berry and Pimentel | JCPSA6-1969-51-2274 (r. p.) |
| Klimek and Berry | ACSRAL-1973-166-Phys. 103 |
| Klimek and Berry | CHPLBC-1973-20-141 |
| Kompa, K. L. | ACIEAY-1970-9-773 (rev.) |
| Pimentel, G. C. | IEJQA7-1970-6-174 (rev.) |

B. $HF^{\ddagger}(DF^{\ddagger})$ Energy Transfer and Quenching

1. $HF^{\ddagger}(DF^{\ddagger})$ Energy Transfer

a. $HF(v_i = 0) + M^{\ddagger} \rightarrow HF^{\ddagger}(v_j > 0) + M$ ($M \neq HF$) (energy transferred to HF from M^{\ddagger})

| | |
|-------------------|-----------------------|
| Hancock and Green | JCPSA6-1972-56-2474 |
| Heydtmann, et al. | AOPAI-1971-10-1755 |
| Suchard, et al. | XADRCA-1973-AD 763716 |

b. $HF^{\ddagger}(v_i = m) + M \rightarrow HF^{(\ddagger)}(v_j < m) + M^{\ddagger} (v_j \geq 0)$
(energy transferred from HF^{\ddagger} to M)

| | |
|-----------------------|-----------------------------|
| Ahl and Cool | JCPSA6-1973-58-5540 |
| Basov, et al. | AOPAI-1971-10-1814 |
| Basov, et al. | JTPLA2-1969-9-375 (r. p.) |
| Basov, et al. | IEJQA7-1970-6-183 (r. p.) |
| Berend and Thommarson | IEJQA7-1973-9-195 |
| Berend and Thommarson | XADRCA-1973-AD 763817 |
| Blauer, et al. | SYMCAQ-1971-13-109 |
| Blauer, et al. | JCPSA6-1972-57-3277 |
| Bott and Cohen | JCPSA6-1973-58-4539 |
| Bott and Cohen | JCPSA6-1973-59-447 |
| Chester, A. N. | JCPSA6-1970-53-3595 (r. p.) |
| Cohen, N. | XADRCA-1972-AD 763715 |
| Cohen, et al. | IEJQA7-1970-6-168 (r. p.) |
| Cool, et al. | APPLAB-1969-15-318 (r. p.) |
| Cool, et al. | JAPIAU-1970-41-4038 |

Dillon and Stephenson
 Falk, T. J.
 Green and Hancock
 Gross, R. W. F.
 Hancock and Green
 Hancock and Green
 Herbelin and Cohen
 Hinchin, J. J.
 Kapralova, et al.
 Kapralova, et al.
 Kerber, et al.
 Kerber, et al.
 Kerber and Whittier
 Sentman, L. H.
 Sentman and Solomon
 Stephens and Cool
 Suchard, et al.
 Vasil'ev, et al.
 Vedeneev, et al.
 Vedeneev, et al.

JCPSA6-1973-58-2056 (calc., cr. sect.)
 XCCIAV-1972-AD 745450
 IEJQA7-1973-9-50
 JCPSA6-1969-50-1889 (r. p.)
 JCPSA6-1972-56-2474
 JCPSA6-1972-57-4515
 CHPLBC-1973-20-605 (r. p.)
 JCPSA6-1973-59-233
 DKPCAG-1971-197-281 (calc.)
 DKPCAG-1971-198-452 (r. p.)
 IEJQA7-1973-9-94 (rev.)
 IEJQA7-1973-9-190 (r. p.)
 *ASTSZx-1970-TOR-0059(6753-10)-1 (calc.)
 CHPLBC-1973-18-493 (calc.)
 JCPSA6-1973-59-89 (calc.)
 JCPSA6-1972-56-5863
 JCPSA6-1972-57-5065
 SPHJAR-1972-34-51
 RJPCAR-1969-43-713
 KICAA8-1970-11-26 (rev.)

c. $HF(v_i) + HF(v_j) \rightarrow HF(v_k) + HF(v_l) \quad (i + j = k + l)$
 (HF - HF energy transfer)

Ahl and Cool
 Berend and Thommarson
 Bott, J. F.
 Bott, J. F.
 Pott and Cohen
 Cohen, N.
 Emanuel, et al.
 Green and Hancock
 Hinchin, J. J.
 Kerber, et al.
 Kerber and Whittier
 Kerber, et al.
 Kompa, et al.
 Osgood, et al.
 Osgood, et al.
 Sentman, L. H.
 Suchard, et al.
 Suchard, et al.

JCPSA6-1973-58-5540
 XADRCA-1973-AD 763817
 IEJQA7-1973-9-189
 JCPSA6-1972-57-96
 JCPSA6-1973-59-447
 XADRCA-1972-AD 763715
 XADRCA-1972-AD 746685 (rev.)
 IEJQA7-1973-9-50
 JCPSA6-1973-59-233
 IEJQA7-1973-9-190
 *ASTSZx-1970-TOR-0059(6753-10)-1
 IEJQA7-1973-9-94 (rev.)
 JCPSA6-1968-49-4257
 IEJQA7-1973-9-190
 APPLAB-1972-20-469
 CHPLBC-1973-18-493 (calc.)
 JCPSA6-1972-57-5065
 XADRCA-1973-AD 763716

2. $HF^\ddagger(DF^\ddagger)$ Quenching

- a. $HF^\ddagger(v_i = m) + M \rightarrow HF^\ddagger(v_j < m) + M \quad (v \geq 0)$
(collisional quenching)

| | |
|-----------------------|--|
| Ahl and Cool | JCPSA6-1973-58-5540 |
| Airey, J. R. | IJCKBO-1970-2-65 |
| Airey and Fried | CHPLBC-1971-8-23 |
| Airey and Smith | JCPSA6-1972-57-1669 |
| Anlauf, et al. | JCPSA6-1973-58-5354 |
| Berend and Thommarson | IEJQA7-1973-9-195 |
| Berend and Thommarson | JCPSA6-1973-58-3454 (calc., traj.) |
| Blair, et al. | JCPSA6-1973-59-1582 |
| Blauer and Solomon | IJCKBO-1973-5-553 |
| Blauer and Solomon | SYMCAQ-1973-14-189 |
| Blauer, et al. | IJCKBO-1972-4-293 |
| Blauer, et al. | XCCIAV-1972-AD 738296 |
| Bott and Cohen | JCPSA6-1971-55-3698 |
| Bott and Cohen | JCPSA6-1971-55-51 4 |
| Bott and Cohen | JCPSA6-1973-58-934 |
| Bott and Cohen | JCPSA6-1973-58-4539 |
| Brokaw, R. S. | JPCHAX-1965-69-2488 |
| Cohen, N. | XADRCA-1972-AD 763715 |
| Emanuel, et al. | XADRCA-1972-AD 746685 (rev.) |
| Fried, et al. | IEJQA7-1973-9-59 |
| Green and Hancock | IEJQA7-1973-9-50 |
| Hancock and Green | JCPSA6-1972-56-2474 |
| Hancock and Green | JCPSA6-1972-57-4515 |
| Hess, L. D. | IEJQA7-1973-9-201 (r. p.) |
| Hinchen, J. J. | IEJQA7-1973-9-196 |
| Hinchen, J. J. | JCPSA6-1973-59-233 |
| Just and Rimpel | IEJQA7-1973-9-196 |
| Kapralova and Chaikin | CBFMAO-1969-13-557 |
| Kapralova, et al. | KICAA8-1969-10-23 |
| Kapralova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Kapralova, et al. | KICAA8-1964-6-884 |
| Kerber, et al. | IEJQA7-1973-9-190 (r. p.) |
| Kerber and Whittier | *ASTSZx-1970-TOR-0059(6753-10)-1 |
| Kerber, et al. | IEJQA7-1973-9-94 (rev.) |
| Kompa, et al. | JCPSA6-1968-49-4257 |
| Kwok, M. A. | IEJQA7-1973-9-196 |
| Molina and Pimentel | IEJQA7-1973-9-64 |
| Parker, J. V. | IEJQA7-1973-9-189 |
| Sentman, L. H. | CHPLBC-1973-18-493 (calc.) |
| Shin, H. K. | CHPLBC-1972-14-64 (calc.) |
| Suchard, et al. | JCPSA6-1972-57-5065 |
| Suchard, et al. | XADRCA-1973-AD 763715 |
| Thompson, D. L. | JCPSA6-1972-57-4164 (calc., pot surf., traj.) |
| Thompson, D. L. | JCPSA6-1972-57-4170 (calc., traj.) |
| Wilkins, R. L. | JCPSA6-1973-58-3038 (calc., pop. distr., pot. surf., traj.) |
| Wilkins, R. L. | JCPSA6-1973-59-698 |

b. $\text{HF}^\ddagger(\nu_i = m) + \text{HF} \rightarrow \text{HF}^\ddagger(\nu_j < m) + \text{HF}(\nu_j \geq 0)$
 (HF - HF self-quenching)

| | |
|-----------------------|----------------------------|
| Ahl and Cool | JCPA6-1973-58-5540 |
| Airey and Fried | CHPLBC-1971-8-23 |
| Airey and Smith | JCPA6-1972-57-1669 |
| Berend and Thommarson | IEJQA7-1973-9-195 |
| Berend and Thommarson | JCPA6-1973-58-3203 |
| Blair, et al. | JCPA6-1973-59-1582 |
| Blauer, et al. | SYMCAQ-1971-13-109 |
| Bott, J. | IEJQA7-1973-9-189 |
| Bott and Cohen | JCPA6-1971-55-3698 |
| Bott and Cohen | JCPA6-1973-58-934 |
| Bott and Cohen | JCPA6-1973-58-4539 |
| Emanuel, et al. | XADRC-1972-AD 746685 |
| Falk, T. J. | XCCIAV-1972-AD 745450 |
| Fried, et al. | IEJQA7-1973-9-59 |
| Green and Hancock | IEJQA7-1973-9-50 |
| Hancock and Green | JCPA6-1972-56-2474 |
| Hancock and Green | JCPA6-1972-57-4515 |
| Hinchen, J. J. | IEJQA7-1973-9-196 |
| Hinchen, J. J. | JCPA6-1973-59-233 |
| Just and Rimpel | IEJQA7-1973-9-196 |
| Kompa, et al. | JCPA6-1968-49-4257 |
| MacLean and Tregay | XADRC-1971-AD 732927 |
| Molina and Pimentel | IEJQA7-1973-9-64 |
| Sentman, L. H. | CHPLBC-1973-18-493 (calc.) |
| Shin, H. K. | CHPLBC-1971-10-81 (calc.) |
| Shin, H. K. | JCPA6-1973-59-879 (calc.) |
| Solomon, et al. | IJCKBO-1971-3-215 |
| Stephens and Cool | JCPA6-1972-56-5863 |
| Suchard, et al. | JCPA6-1972-57-5065 |
| Tal'roze, et al. | KICAA8-1970-11-233 |
| Thompson, D. L. | JCPA6-1972-57-2589 |
| Vasil'ev, et al. | DKPCAG-1970-191-296 |

c. $\text{HF}^\ddagger(\nu_i = m) + \text{M} \rightarrow \text{products (dissociative quenching)}$

i. $\text{HF}^\ddagger(\nu_i = m) + \text{M}_2 \rightarrow \text{HF}(\nu_j = 0) + \text{M} + \text{M}$

| | |
|-----------------------|-----------------------------|
| Airey, J. R. | IJCKBO-1970-2-65 |
| Basov, et al. | JTPLA2-1969-9-375 (r. p.) |
| Brokaw, R. S. | JCPA6-1965-69-2488 |
| Kapralova and Chaikin | CBFMAO-1969-13-557 |
| Kapralova and Chaikin | KICAA8-1969-10-195 (r. p.) |
| Kapralova, et al. | DKPCAG-1971-198-452 (r. p.) |
| Kapralova, et al. | KICAA8-1969-10-23 |
| Kapralova, et al. | KICAA8-1963-4-567 (r. p.) |
| Kapralova, et al. | KICAA8-1964-6-884 |
| Kompa, K. L. | ACIEAY-1970-9-773 (rev.) |
| Tal'roze, et al. | KICAA8-1970-11-233 |
| Vasil'ev, et al. | DKPCAG-1970-191-296 |

ii. $HF^{\ddagger}(v_i = m) + M \rightarrow H + F + M$

MacLean and Tregay

SYMCAQ-1973-14-157

C. HF^{\ddagger} (DF^{\ddagger}) Theoretical papers

| | |
|-----------------------|---|
| Anlauf, et al. | JCPSA6-1970-53-4091 (pop. distr.) |
| Ben-Shaul, et al. | JCPSA6-1972-57-5427 (calc., pop. distr.) |
| Ben-Shaul, et al. | CHPLBC-1972-15-160 (pop. distr.) |
| Berend and Thommarson | JCPSA6-1973-58-3454 (calc., traj.) |
| Blais and Truhlar | JCPSA6-1973-58-1090 (pot. surf., traj.) |
| Dillon and Stephenson | JCPSA6-1973-58-2056 (calc., cr. sect.) |
| Emanuel and Whittier | APOPAI-1972-11-2047 (calc.) |
| Jaffe and Anderson | JCPSA6-1971-54-2224 (pot. surf., traj.) |
| Jaffe, et al. | JCPSA6-1973-59-1128 (pot. surf., traj.) |
| Jonathan, et al. | MOPHAM-1972-24-1143 (pop. distr., pot. surf., traj.) |
| Kapralova, et al. | CHPLBC-1968-2-581 (trans. prob.) |
| Kerber, et al. | APOPAI-1972-11-1112 (pop. distr., model.) |
| Levine, et al. | CHPLBC-1973-19-1 (pop. distr.) |
| Muckerman, J. T. | JCPSA6-1971-54-1155 (traj.) |
| Muckerman, J. T. | JCPSA6-1972-56-2997 (pot. surf., traj.) |
| Muckerman, J. T. | JCPSA6-1972-57-3388 (pop. distr., traj.) |
| Muckerman and Newton | JCPSA6-1972-56-3191 (pot. surf.) |
| O'Neil, et al. | JCPSA6-1973-58-1126 (calc., pot. surf.) |
| Polanyi and Sloan | JCPSA6-1972-57-4988 (d. r.) |
| Polanyi and Tardy | JCPSA6-1969-51-5717 (pop. distr.) |
| Polanyi and Woodall | JCPSA6-1972-57-1574 (d. r.) |
| Schatz, et al. | JCPSA6-1973-58-4023 (pop. distr.) |
| Thompson, D. L. | JCPSA6-1972-57-4164 (calc., pot. surf. traj.) |
| Thompson, D. L. | JCPSA6-1972-57-4170 (calc., traj.) |
| Thruhlar, D. G. | JCPSA6-1972-56-3189 (pot. surf.) |
| Wilkins, R. L. | JCPSA6-1972-57-912 (calc., pop. distr., pot. surf., traj.) |
| Wilkins, R. L. | JCPSA6-1973-58-3038 (calc., pop. distr. pot. surf., traj.) |
| Wilkins, R. L. | JCPSA6-1973-58-2326 (calc., pop. distr., pot. surf., traj.) |
| Wilkins, R. L. | JCPSA6-1973-59-698 (calc., d.r., pop. distr., pot. surf., traj.) |

Part II. Hydrogen chloride (HCl, DCl)

A. Formation of HCl^\ddagger (DCl^\ddagger)

1. Bimolecular reactions (abstraction lasers)

a. Abstraction of H(D) atom by Cl atom

i. $\text{Cl} + \text{H}_2 \rightarrow \text{HCl}^\ddagger + \text{H}$

| | |
|------------------------|-----------------------------|
| Ashmore, P. G. | TFSOA4-1953-49-251 (r. p.) |
| Ashmore and Chanmugam | TFSOA4-1953-49-254 (r. p.) |
| Benson, et al. | IJCKBO-1969-1-29 (r. p.) |
| Clyne and Walker | JCFAR-1973-69-1547 (r. p.) |
| Corneil, P. H. | DABSA9-1968-28-4524 |
| Corneil and Kasper | IEJQA7-1970-6-170 |
| Corneil and Pimentel | JCPSA6-1968-49-1379 |
| Davis, et al. | IJCKBO-1970-2-101 (r. p.) |
| Deutsch, T. F. | APPLAB-1967-10-234 (r. p.) |
| Deutsch, T. F. | APPLAB-1967-11-13 (r. p.) |
| Deutsch, T. F. | IEJQA7-1967-3-419 (r. p.) |
| Fettis and Knox | PRKNAZ-1964-2-2 (r. p.) |
| Galante and Gislason | CHPLBC-1973-18-231 (r. p.) |
| Henry, et al. | CHDBAN-1968-267-616 |
| Johnson, et al. | JCPSA6-1970-52-6372 |
| Klein, et al. | JCPSA6-1964-41-1799 |
| Kompa, K. L. | CITEAH-1970-42-573 (rev.) |
| Norrish, R. G. W. | PRLAAZ-1967-301-1 (r. p.) |
| Pimentel, G. C. | SCAMAC-1966-214-32 (r. p.) |
| Raff, et al. | JCPSA6-1970-53-1606 |
| Shizgal and Karplus | JCPSA6-1971-54-4357 (r. p.) |
| Snider, N. S. | JCPSA6-1970-53-4116 (r. p.) |
| Stedman, et al. | CHPLBC-1970-7-173 |
| Truhlar, D. G. | JCPSA6-1972-56-3189 (r. p.) |
| Westenberg, A. A. | JCPSA6-1970-53-4117 (r. p.) |
| Westenberg and de Haas | JCPSA6-1968-48-4405 (r. p.) |
| Wood, G. O. | JCPSA6-1972-56-1723 (r. p.) |
| Wood and Chang | APPLAB-1972-20-77 (r. p.) |
| Yaakov, et al. | JCPSA6-1973-59-2415 (r. p.) |

ii. $\text{Cl} + \text{HX} \rightarrow \text{HCl}^\ddagger + \text{X}$

| | |
|-------------------|----------------------------------|
| Airey, J. P. | IEJQA7-1967-3-203 (r. p.) |
| Airey, J. R. | IEJQA7-1970-6-175 |
| Airey, J. R. | JCPSA6-1970-52-156 |
| Anlauf, et al. | JCPSA6-1970-53-4091 |
| Anlauf, et al. | DFSOAW-1967-44-183 (pop. distr.) |
| Anlauf, et al. | PYLAAG-1967-24-208 (pop. distr.) |
| Anlauf, et al. | JCPSA6-1968-49-5189 (calc.) |
| Ben-Shaul, et al. | CHPLBC-1972-15-160 (pop. distr.) |
| Ben-Shaul, et al. | JCPSA6-1972-57-5427 (calc.) |
| Blauer, et al. | XADRCA-1972-AD 738296 |
| Chester, A. N. | JCPSA6-1970-53-3595 |
| Cool, et al. | APPLAB-1969-15-313 (r. p.) |

Cool, et al.
Cool, et al.
Cowley, et al.
Glaze, et al.
Kompa, K. L.
Levine, et al.
Maylotte, et al.
Moore, C. B.
Moore and Zittel
Naegeli and Ultee
Pimentel, G. C.
Polanyi, J. C.
Polanyi and Woodall

IJCKBO-1969-1-495 (r. p.)
JAPIAU-1970-41-4038 (r. p.)
CHPLBC-1971-12-144
APPLAB-1971-18-173 (r. p.)
ACIEAY-1970-9-773 (rev.)
CHPLBC-1973-19-1 (pop. distr.)
JCPSA6-1972-57-1547
IEJQA7-1968-4-52 (r. p.)
SCIEAS-1973-182-541 (rev.)
CHPLBC-1970-6-121 (r. p.)
PACHAS-1969-18-275 (rev.)
APOSAR-1965-2-109 (theory)
JCPSA6-1972-56-1563 (calc.)

iii. $\text{Cl} + \text{RH} \rightarrow \text{HCl}^\ddagger + \text{R}$

Clyne and Walker
Davis, et al.
Fettis and Knox
Knox and Nelson

JCF TAR-1973-69-1547 (r. p.)
IJCKBO-1970-2-101 (r. p.)
PRKNAZ-1964-2-2 (r. p.)
TF SOA4-1959-55-937

b. Abstraction of Cl Atom by H(D) Atom

i. $\text{H} + \text{Cl}_2 \rightarrow \text{HCl}^\ddagger + \text{Cl}$

Airey, J. R.
Airey, et al.
Airey, et al.
Albright, et al.
Anlauf, K. G.
Anlauf, et al.
Anlauf, et al.
Anlauf, et al.
Anlauf, et al.
Ashmore, P. G.
Basov, et al.
Ben-Shaul, et al.
Bowen and Overholser
Cabre and Henry
Cabre and Henry
Charters, et al.
Cashion and Polanyi
Cashion and Polanyi
Cashion and Polanyi
Cashion and Polanyi
Charters and Polanyi
Chester, A. N.
Cool, et al.
Cool, et al.
Corneil and Kasper
Dodonov, et al.

IJCKBO-1970-2-65
CJCHAG-1964-42-2193
JCPSA6-1964-41-3255
JCPSA6-1969-50-3632
DABBA-1970-31-1195 (calc., pop. distr.)
JCPSA6-1970-53-4091 (calc., pop. distr.)
JCPSA6-1972-57-1561 (d. r.)
DFSOAW-1967-44-183 (pop. distr.)
PYLAAG-1967-24-208 (pop. distr.)
TF SOA4-1953-49-251 (mech.)
JTPLA2-1969-9-147 (rev.)
JCPSA6-1972-57-5427 (calc., pop. distr.)
ASACAW-1969-14-475 (pop. distr.)
JCPQAY-1967-64-119 (pop. distr.)
CHDBAN-1969-269-46 (pop. distr.)
NATUAS-1962-193-367 (r. p.)
JCPSA6-1958-29-455 (r. p.)
JCPSA6-1959-30-1097 (pop. distr.)
JCPSA6-1961-35-600
PRLAAZ-1960-258-529 (pop. distr.)
PRLAAZ-1960-258-564 (r. p.)
DFSOAW-1962-33-107 (pop. distr.)
JCPSA6-1970-53-3595 (calc., pop. distr.)
APPLAB-1969-15-318 (r. p.)
JAPIAU-1970-41-4038 (r. p.)
IEJQA7-1970-6-170
KICAA8-1970-11-677

Fass, et al.
 Henry, et al.
 Kasper, J. V. V.
 Kasper and Pimentel
 Klein and Wolfsberg
 Kompa, K. L.
 Levine, et al.
 Mayer, et al.
 Ménard-Bourcin, et al.
 Miller and Light
 Moore, C. B.
 Norrish, R. G. W.
 Pacey and Polanyi
 Perona, et al.
 Pimentel, G. C.
 Pimentel, G. C.
 Pimentel, G. C.
 Pimentel, G. C.
 Polanyi, J. C.
 Polanyi, J. C.
 Polanyi, J. C.
 Polanyi, J. C.
 Polanyi, J. C.
 Polanyi, J. C.
 Polanyi, J. C.
 Polanyi and Rosner
 Polanyi and Woodall
 Rice and Jensen
 Russell and Light

JPCHAX-1972-76-2801 (r. p.)
 CHDBAN-1968-267-616
 DIASA9-1966-26-5062 (r. p.)
 PRLTAO-1965-14-352
 JCPSA6-1961-34-1494 (r. p.)
 CITEAH-1970-42-573 (rev.)
 CHPLBC-1973-19-1 (pop. dist.)
 SYMCAQ-1967-11-837 (r. p.)
 CHDBAN-1972-274-241 (pop. distr.)
 JCPSA6-1971-54-1643 (calc., pot. surf.)
 IEJQA7-1968-4-52 (r. p.)
 PRLAAZ-1967-301-1 (r. p.)
 APOPAI-1971-10-1725
 JCPSA6-1970-52-6384
 DAKAAT-1969-50-1 (rev.)
 IEJQA7-1970-6-174 (rev.)
 PACHAS-1969-18-275 (rev.)
 SCAMAC-1966-214-32 (r. p.)
 APOSAR-1965-2-109 (calc., pop. distr.)
 CHMBAY-1966-2-151 (rev.)
 DFSOAW-1962-33-279 (r. p.)
 IEJQA7-1970-6-168 (r. p.)
 JCPSA6-1959-31-1338 (rev.)
 JCPSA6-1961-34-347 (calc., pop. distr.)
 JQSRAE-1963-3-471 (rev.)
 JCPSA6-1963-38-1028 (r. p.)
 JCPSA6-1972-56-1563 (cal., pop. distr.)
 IEJQA7-1973-9-199
 JCPSA6-1969-51-1720 (calc., pop. distr.,
 traj.)
 KICAA8-1964-6-1 (r. p.)
 BSCBAG-1958-67-135 (r. p.)
 IEJQA7-1970-6-169 (r. p.)
 CHPLBC-1970-7-173
 JCPSA6-1965-42-806 (r. p.)
 ACIEAY-1971-10-604 (rev.)

ii. $H + ClX \rightarrow HCl^{\frac{1}{2}} + X$

Anlauf, et al.
 Krogh and Pimentel
 Mayer, et al.

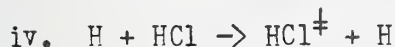
JCPSA6-1970-53-4091 (calc. pop. distr.)
 JCPSA6-1972-56-969
 SYMCAQ-1967-11-837 (r. p.)

iii. $H + RCl \rightarrow HCl^{\frac{1}{2}} + R$

Anlauf, K. G.
 Charters, et al.
 Cabre and Henry
 Cashion and Polanyi
 Freeman and Phillips
 Henry, et al.
 Heydtmann and Polanyi

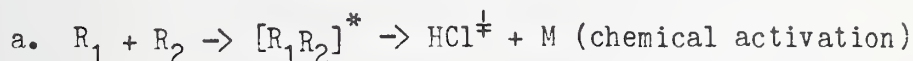
DABBBA-1970-31-1195 (pop. distr.)
 NATUAS-1962-193-367 (r. p.)
 CHDBAN-1969-269-46 (pop. distr.)
 JCPSA6-1961-35-600
 JPCHAX-1968-72-3031 (r. p.)
 CHDBAN-1968-267-616
 APOPAI-1971-10-1738 (pop. distr.)

| | |
|------------------------|-----------------------------------|
| Johnson, R. L. | DABBA-1969-30-2632 (pop. distr.) |
| Johnson, et al. | JCPA6-1970-52-6372 (pop. distr.) |
| Johnson and Setser | CHPLBC-1969-3-207 (pop. distr.) |
| Lin, M. C. | CHPLBC-1970-7-209 (mech.) |
| Ménard-Bourcin, et al. | CHDBAN-1972-274-241 (pop. distr.) |
| Perona, et al. | JCPA6-1970-52-6384 |
| Perona, et al. | JPCA6-1969-73-2091 |
| Rabideau, S. W. | JCPA6-1973-59-1533 |
| Rice and Jensen | IEQA7-1973-9-199 |

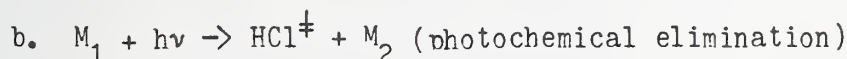


| | |
|---------------------|-----------------------------------|
| Cashion and Polanyi | PRLAAZ-1960-258-529 (pop. distr.) |
| Wood, G. O. | JCPA6-1972-56-1723 (r. p.) |

2. Unimolecular Reactions (elimination lasers)



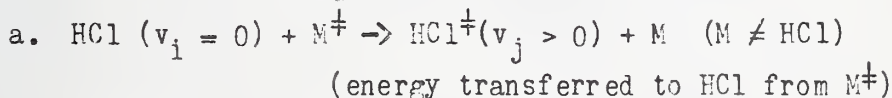
| | |
|--------------------|----------------------------------|
| Berry and Pimentel | IEQA7-1970-6-176 |
| Chang, et al. | JPCA6-1971-75-2070 (pop. distr.) |
| Lin, M. C. | IEQA7-1973-9-200 (r. p.) |



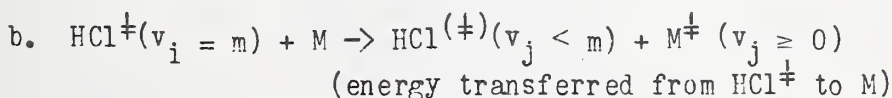
| | |
|---------------------|--------------------|
| Berry, M. J. | DABBA-1971-31-7210 |
| Berry and Pimentel | IEQA7-1970-6-176 |
| Berry and Pimentel | JCPA6-1969-51-2274 |
| Berry and Pimentel | JCPA6-1970-53-3453 |
| Molina and Pimentel | IEQA7-1973-9-64 |
| Molina and Pimentel | JCPA6-1972-56-3988 |

B. $HCl^{\ddagger}(DCl^{\ddagger})$ Energy Transfer and Quenching

1. $HCl^{\ddagger}(DCl^{\ddagger})$ Energy transfer



| | |
|------------------|----------------------------|
| Ahl and Cool | JCPA6-1973-58-5540 |
| Blauer, et al. | JCPA6-1972-57-3277 |
| Chen, et al. | CHPLBC-1968-2-593 |
| Moore and Zittel | SCIEAS-1973-182-541 (rev.) |



| | |
|----------------------|--------------------|
| Ahl and Cool | JCPA6-1973-58-5540 |
| Airey, J. R. | IEQA7-1970-6-175 |
| Airey, J. R. | JCPA6-1970-52-156 |
| Bott and Cohen | JCPA6-1973-58-4539 |
| Powen and Overholser | ASACAW-1969-14-475 |
| Chen and Moore | IEQA7-1970-6-175 |

| | |
|-----------------------|--|
| Chen and Moore | JCPSA6-1971-54-4072 |
| Chen and Moore | JCPSA6-1971-54-4080 |
| Chen, et al. | CHPLBC-1968-2-593 |
| Cool, et al. | IJCKBO-1969-1-495 (r. p.) |
| Cool, et al. | JAPIAU-1970-41-4038 (r. p.) |
| Dillon and Stephenson | JCPSA6-1973-58-2056 (calc., cr. sect.) |
| Hopkins, et al. | JCPSA6-1973-59-836 |
| Hopkins and Chen | JCPSA6-1972-57-3161 |
| Moore, C. B. | ACHRAY-1969-2-103 (rev.) |
| Moore and Zittel | SCIEAS-1973-182-541 (rev.) |
| Sentman, L. H. | CHPLBC-1973-18-493 (calc., model.) |
| Stephenson, et al. | JCPSA6-1972-56-5214 |
| Zittel and Moore | JCPSA6-1973-58-2004 |

- c. $\text{HCl}(v_i) + \text{HCl}(v_j) \rightarrow \text{HCl}(v_k) + \text{HCl}(v_l) \quad (i + j = k + l)$
(HCl - HCl energy transfer)

| | |
|-----------------------|------------------------------------|
| Bowen and Overholser | ASACAW-1969-14-475 |
| Chen and Moore | JCPSA6-1971-54-4072 |
| Chen and Moore | JCPSA6-1971-54-4080 |
| Chen, et al. | CHPLBC-1968-2-593 |
| Cohen, et al. | IJCKBO-1969-1-551 |
| Corneil and Kasper | IEJQA7-1970-6-170 (calc.) |
| Findlay and Polanyi | CJCHAG-1964-42-2176 |
| Findlay and Polanyi | DFSOAW-1962-33-274 |
| Gorshkov, et al. | APOPAI-1971-10-1781 |
| Hopkins and Chen | IEJQA7-1973-9-196 |
| Hopkins and Chen | JCPSA6-1972-57-3816 |
| Izoshin and Oraevskii | HIECAP-1971-5-357 (calc.) |
| Leone and Moore | CHPLPC-1973-19-340 |
| Moore and Zittel | SCIEAS-1973-182-541 (rev.) |
| Polanyi, J. C. | JQSRAE-1963-3-471 (rev.) |
| Sentman, L. H. | CHPLBC-1973-18-493 (calc., model.) |
| Sharma, et al. | JCPSA6-1973-58-3519 (calc.) |

2. $\text{HCl}^{\pm}(\text{DCI}^{\pm})$ Quenching

- a. $\text{HCl}^{\pm}(v_i = m) + M \rightarrow \text{HCl}^{\pm}(v_j < m) + M \quad (v_j \geq 0)$ (collisional quenching)

| | |
|----------------------|---|
| Ahl and Cool | JCPSA6-1973-58-5540 |
| Bott and Cohen | JCPSA6-1973-58-4539 |
| Bowen and Overholser | ASACAW-1969-14-475 |
| Chen and Moore | JCPSA6-1971-54-4072 |
| Chen, et al. | CHPLBC-1968-2-593 |
| Cohen, et al. | IJCKBO-1969-1-551 |
| Corneil and Kasper | IEJQA7-1970-6-170 (calc.) |
| Craig and Moore | JPCHAX-1971-75-1622 |
| Gorshkov, et al. | APOPAI-1971-10-1781 |
| Hopkins and Chen | JCPSA6-1972-57-3161 |
| Kapralova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Letokhov, V. S. | SCIEAS-1973-180-451 |

Moore and Zittel
 Ridley and Smith
 Ridley and Smith
 Seery, D. J.
 Sentman, L. H.
 Smith and Wood
 Zittel and Moore

SCIEAS-1973-182-541 (rev.)
 CHPLBC-1971-9-457
 JCFTBS-1972-68-1231
 JCPSA6-1973-58-1796
 CHPLBC-1973-18-493 (calc., model.)
 MOPHAM-1973-25-441
 JCPSA6-1973-58-2004



(HCl - HCl self-quenching)

Ahl and Cool
 Borrell, P.
 Bowen and Overholser
 Bowman and Seery
 Breazeale and Kneser
 Breshears and Bird
 Cabre and Henry
 Chen, H-L.
 Chen and Moore
 Chen, et al.
 Cohen, et al.
 Corneil, P. H.
 Corneil and Kasper
 Ferguson and Read
 Kapralova, et al.
 Letokhov, V. S.
 Margottin-Maclou, et al.
 Molina and Pimentel
 Moore, C. B.
 Ridley and Smith
 Sentman, L. H.
 Shin, H. K.
 Shin, H. K.
 Stephenson, et al.
 Thommarson and Berend

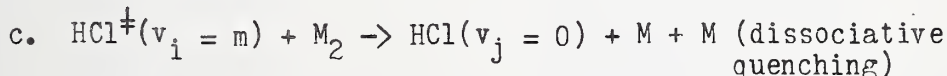
JCPSA6-1973-58-5540
 CSSPAD-1966-20-263
 ASACAW-1969-14-475
 JCPSA6-1969-50-1904
 JASMAN-1960-32-885
 JCPSA6-1969-50-333
 JCPQAY-1967-64-119 (pop. distr.)
 JCPSA6-1971-55-5551
 JCPSA6-1971-54-4072
 CHPLBC-1968-2-593
 IJCKBO-1969-1-551
 DABSA9-1968-28-4524 (r. p.)
 IEJQA7-1970-6-170
 TFSOA4-1967-63-61 (calc.)
 CHPLBC-1968-2-581 (calc., trans. prob.)
 SCIEAS-1973-180-451
 APOPAI-1971-10-1768
 IEJQA7-1973-9-64
 JCPSA6-1965-43-297 (calc., model.)
 JCFTBS-1972-68-1231
 CHPLBC-1973-18-493 (calc., model.)
 CHPLBC-1970-6-494 (calc.)
 JPCHAX-1971-75-1079 (calc.)
 JCPSA6-1972-56-5214
 IJCKBO-1973-5-629 (calc., pot. surf.,
 traj.)

Thompson, D. L.

JCPSA6-1972-56-3570 (calc., pot. surf.,
 traj.)

Thompson, D. L.
 Zittel and Moore

JCPSA6-1972-57-2589
 JCPSA6-1973-58-2004



Anlauf, et al.
 Sloodmaekers and Van Tiggelen

JCPSA6-1969-51-5716
 BSCBAG-1958-67-135 (r. p.)

C. HCl^\ddagger (DCl^\ddagger) Theoretical papers

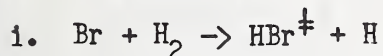
| | |
|-----------------------|--|
| Anlauf, et al. | JCPA6-1970-53-4091 (calc., pop. distr.) |
| Anlauf, et al. | JCPA6-1972-57-1561 (calc., d. r.) |
| Anlauf, et al. | JCPA6-1968-49-5189 (pop. distr.) |
| Ben-Shaul, et al. | CHPLBC-1972-15-160 (pop. distr.) |
| Ben-Shaul, et al. | JCPA6-1972-57-5427 (calc., pop. distr.) |
| Dillon and Stephenson | JCPA6-1973-58-2056 (calc., cr. sect.) |
| Kapralova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Levine, et al. | CHPLBC-1973-19-1 (pop. distr.) |
| Miller and Light | JCPA6-1971-54-1643 (calc., pot. surf.) |
| Moore, C. B. | JCPA6-1965-43-2979 (calc., model.) |
| Parr and Truhlar | JPCHAX-1971-75-1344 (calc., pot. surf.) |
| Parr, et al. | JCPA6-1973-58-5 (calc., pop. distr., pot. surf., traj.) |
| Polanyi, J. C. | APOSAR-1965-2-109 (pot. surf.) |
| Polanyi, J. C. | JCPA6-1959-31-1338 (pop. distr.) |
| Polanyi and Rosner | JCPA6-1963-38-1028 (r. p.) |
| Polanyi and Woodall | JCPA6-1972-56-1563 (calc., pop. distr.) |
| Raff, et al. | JCPA6-1970-53-1606 (calc.) |
| Rankin and Light | JCPA6-1969-51-1701 (calc., pop. distr., pot. surf.) |
| Russell and Light | JCPA6-1969-51-1270 (calc., pop. distr., traj.) |
| Sentman, L. H. | CHPLBC-1973-18-493 (calc., model.) |
| Sharma, et al. | JCPA6-1973-58-3519 (calc.) |
| Shin, H. K. | CHPLBC-1970-6-494 (calc., model.) |
| Shin, H. K. | JPCHAX-1971-75-1079 (calc.) |
| Stern, et al. | JCPA6-1973-58-5697 (calc., model.) |
| Wei and Yankwich | JCPA6-1973-58-5552 (calc.) |

Part III. Hydrogen bromide (HBr, DBr)

A. Formation of HBr^\ddagger (DBr^\ddagger)

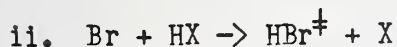
1. Bimolecular reactions (abstraction lasers)

a. Abstraction of H (D) atom by Br atom



Bodenstein and Jung
Deutsch, T. F.
Deutsch, T. F.
Fettis and Knox
Jost, W.
Raff, et al.
Truhlar, D. G.
Wood and Chang

ZEPCAC-1926-121-127 (r. p.)
APPLAB-1967-10-234 (r. p.)
IEJQA7-1967-3-419 (r. p.)
PRKNAZ-1964-2-2 (r. p.)
ZPCBAL-1929-3-95 (r. p.)
JCPSA6-1970-53-1606 (calc.)
JCPSA6-1972-56-3189 (pot. surf.)
APPLAB-1972-20-77 (r. p.)



Anlauf, et al.
Blauer, et al.
Maylotte, et al.

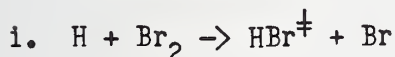
DFSOAW-1967-44-183 (calc.)
XADRC-1972-AD 738296
JCPSA6-1972-57-1547 (pop. distr.)



Fettis and Knox

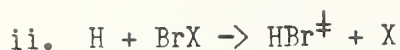
PRKNAZ-1964-2-2 (r. p.)

b. Abstraction of Br Atom by H(D) Atom



Airey, et al.
Anlauf, K. G.
Anlauf, et al.
Anlauf, et al.
Anlauf, et al.
Anlauf, et al.
Ben-Shaul, et al.
Bodenstein and Jung
Cashion and Polanyi
Chester, A. N.
Cool and Stephens
Fass, et al.
Jost, W.
Mayer, et al.
Pimentel, G. C.
Polanyi, J. C.
Polanyi, J. C.
Wagner and Wolfrum
White, J. M.

SYMCAQ-1967-11-85
DABEBA-1970-31-1195
JCPSA6-1970-53-4091 (calc., pop. distr.)
JCPSA6-1972-57-1561 (calc., d. r.)
DFSOAW-1967-44-183 (calc., pop. distr.)
PYLAAG-1967-24-208 (pop. distr.)
JCPSA6-1972-57-5427 (calc., pop. distr.)
ZEPCAC-1926-121-127 (r. p.)
PRLAAZ-1960-258-570
JCPSA6-1970-53-3595 (calc., pop. distr.)
JCPSA6-1970-52-3304 (r. p.)
JPCHAX-1972-76-2801
ZPCBAL-1929-3-95 (r. p.)
SYMCAQ-1967-11-837 (r. p.)
PACHAS-1969-18-275 (rev.)
IEJQA7-1970-6-168 (r. p.)
JCPSA6-1959-31-1338 (rev.)
ACIEAY-1971-10-604 (rev.)
JCPSA6-1973-58-4482 (calc., cr. sec.,
pop. distr., traj.)

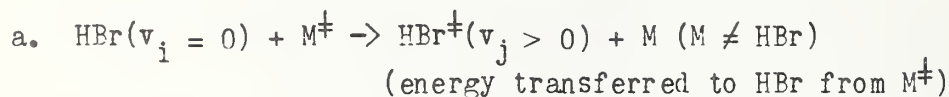


Ben-Shaul, et al.
Mayer, et al.

JCPA6-1972-57-5427 (calc., pop. distr.)
SYMCAQ-1967-11-837 (r. p.)

B. $HBr^{\ddagger} (DBr^{\ddagger})$ Energy Transfer and Quenching

1. $HBr^{\ddagger} (DBr^{\ddagger})$ Energy Transfer



Ahl and Cool

JCPA6-1973-58-5540

Airey, J. R.

IEJQA7-1970-6-175

Airey, J. R.

JCPA6-1970-52-156

Bott and Cohen

JCPA6-1973-58-4539

Chen and Moore

IEJQA7-1970-6-175

Chen and Moore

JCPA6-1971-54-4080

Cool, et al.

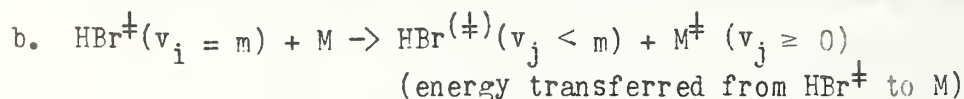
JAPIAU-1970-41-4038

Donovan, et al.

TFSOA4-1970-66-2148

Moore and Zittel

SCIEAS-1973-182-541 (rev.)



Ahl and Cool

JCPA6-1973-58-5540

Bott and Cohen

JCPA6-1973-58-4539

Chen, H-L.

JCPA6-1971-55-5551

Chen, H-L.

JCPA6-1971-55-5557

Cool and Stephens

JCPA6-1970-52-3304 (r. p.)

Donovan, et al.

TFSOA4-1970-66-2148

Hopkins, et al.

JCPA6-1973-59-836

Hopkins and Chen

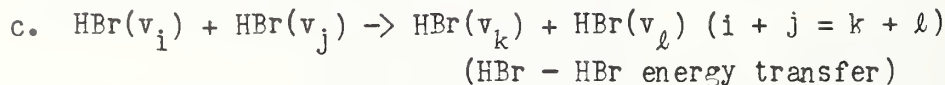
JCPA6-1973-59-1495

Sentman, L. H.

CHPLBC-1973-18-493 (calc., model.)

Stephenson, et al.

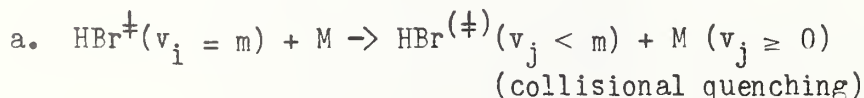
JCPA6-1972-56-5214



Chen, H-L.

JCPA6-1971-55-5551

2. $HBr^{\ddagger} (DBr^{\ddagger})$ Quenching



Ahl and Cool

JCPA6-1973-58-5540

Bott and Cohen

JCPA6-1973-58-4539

Chen and Chen

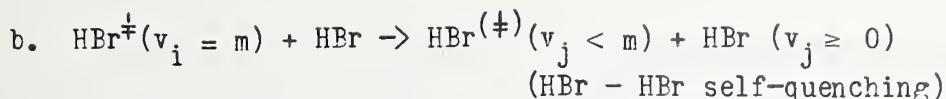
JCPA6-1972-56-3315

Hopkins and Chen

JCPA6-1973-59-1495

Sentman, L. H.

CHPLBC-1973-18-493 (calc., model.)



| | |
|--------------------|---|
| Ahl and Cool | JCPA6-1973-58-5540 |
| Borrell, P. | CSSPAD-1966-20-263 |
| Breshears and Bird | JCPA6-1970-52-999 |
| Chen and Chen | JCPA6-1972-56-3315 |
| Ferguson and Read | TFSOA4-1967-63-61 |
| Kapralova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Kiefer, et al. | JCPA6-1969-50-3641 |
| Moore, C. B. | JCPA6-1965-43-2979 (calc., model.) |
| Sharma, et al. | JCPA6-1973-58-3519 (calc.) |
| Shin, H. K. | JPCHAX-1971-75-1079 (calc.) |
| Shin, H. K. | JCPA6-1968-49-3964 (r. p.) |
| Stephenson, et al. | JCPA6-1972-56-5214 |

c. $\text{HBr}^{\ddagger}(\text{DBr}^{\ddagger})$ Theoretical papers

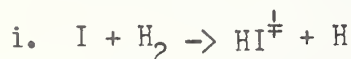
| | |
|-------------------|---|
| Anlauf, et al. | JCPA6-1972-57-1561 (d. r.) |
| Ben-Shaul, et al. | JCPA6-1972-57-5427 (calc., pop. distr.) |
| Chester, A. N. | JCPA6-1970-53-3595 (calc.) |
| Kapralova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Moore, C. B. | JCPA6-1965-43-2979 (calc., model.) |
| Parr and Truhlar | JPCHAX-1971-75-1844 (calc., pot. surr.) |
| Pirkle and McGee | JCPA6-1968-49-3532 (calc., cr. sect., pot. surr.) |
| Polanyi, J. C. | JCPA6-1959-31-1338 (rev.) |
| Raff, et al. | JCPA6-1970-53-1606 (calc.) |
| Sentman, L. H. | CHPLBC-1973-18-493 (calc., model.) |
| Sharma, et al. | JCPA6-1973-58-3519 (calc.) |
| Shin, H. K. | JPCHAX-1971-75-1079 (calc.) |
| Shin, H. K. | JCPA6-1968-49-3964 (r. p.) |
| White, J. M. | JCPA6-1973-58-4482 (calc., cr. sec., pop. distr., traj.) |

Part IV. Hydrogen iodide (HI, DI)

A. Formation of $\text{HI}^\ddagger(\text{DI}^\ddagger)$

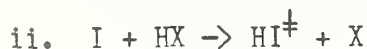
1. Bimolecular Reactions (abstraction lasers)

a. Abstraction of H(D) Atom by I Atom



Fettis and Knox
Henry, et al.
Parr and Truhlar
Raff, et al.
Truhlar, D. G.

PRKNAZ-1964-2-2 (r. p.)
CHPLBC-1973-20-138 (r.p., traj.)
JPCHAX-1971-75-1844 (calc., pot. surf.)
JCPSA6-1970-53-1606 (calc.)
JCPSA6-1972-56-3189 (pot. surf.)



Anlauf, et al.

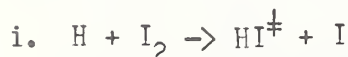
JCPSA6-1969-51-5716



Wagner and Wolfrum

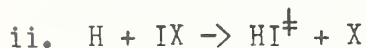
ACIEAY-1971-10-604 (rev.)

b. Abstraction of I Atom by H(D) Atom



Anderson and Kung
Ben-Shaul, et al.
Mayer, et al.
Penzhorn and Darwent
Sullivan, J. H.

JCPSA6-1973-58-2477 (pop. distr., traj.)
JCPSA6-1972-57-5427
SYMCAQ-1967-11-837 (r. p.)
JPCHAX-1968-72-1539 (r. p.)
JCPSA6-1963-39-3001 (r. p.)



Ben-Shaul, et al.
Johnson, et al.

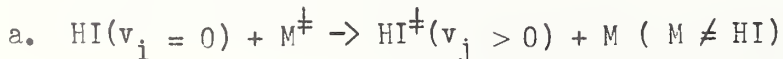
JCPSA6-1972-57-5427 (calc., pop. distr.)
JPCHAX-1973-77-2499 (calc., pot. surf.,
traj.)

Mayer, et al.

SYMCAQ-1967-11-837 (r. p.)

B. $\text{HI}^\ddagger(\text{DI}^\ddagger)$ Energy Transfer and Quenching

1. $\text{HI}^\ddagger(\text{DI}^\ddagger)$ Energy Transfer



(energy transferred to HI from M^\ddagger)

Ahl and Cool
Chen, H-L.
Chen and Moore
Chen, et al.

JCPSA6-1973-58-5540
JCPSA6-1971-55-5551
JCPSA6-1971-54-4080
CHPLBC-1968-2-593

- b. $\text{HI}^{\ddagger}(\nu_i = m) + \text{M} \rightarrow \text{HI}^{\ddagger}(\nu_j < m) + \text{M}^{\ddagger} (\nu_j \geq 0)$
 (energy transferred from HI^{\ddagger} to M)

| | |
|--------------------|---------------------|
| Ahl and Cool | JCPSA6-1973-58-5540 |
| Breshears and Bird | JCPSA6-1971-54-2968 |
| Chen, H-L. | JCPSA6-1971-55-5551 |
| Stephenson, et al. | JCPSA6-1972-56-5214 |

- c. $\text{HI}(\nu_i) + \text{HI}(\nu_j) \rightarrow \text{HI}(\nu_k) + \text{HI}(\nu_l) (i + j = k + l)$
 (HI - HI energy transfer)

| | |
|-----------------|------------------------------------|
| Chow and Greene | JCPSA6-1965-43-324 |
| Sentman, L. H. | CHPLBC-1973-18-493 (calc., model.) |

2. $\text{HI}^{\ddagger}(\text{DI}^{\ddagger})$ Quenching

- a. $\text{HI}^{\ddagger}(\nu_i = m) + \text{M} \rightarrow \text{HI}^{\ddagger}(\nu_j < m) + \text{M} (\nu_j \geq 0)$
 (collisional quenching)

| | |
|--------------------|---|
| Ahl and Cool | JCPSA6-1973-58-5540 |
| Breshears and Bird | JCPSA6-1971-54-2968 |
| Chen, H-L. | JCPSA6-1971-55-5551 |
| Chow and Greene | JCPSA6-1965-43-324 |
| Kapralova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Kiefer, et al. | JCPSA6-1969-50-3641 |

- b. $\text{HI}^{\ddagger}(\nu_i = m) + \text{HI} \rightarrow \text{HI}^{\ddagger}(\nu_j < m) + \text{HI} (\nu_j \geq 0)$
 (HI - HI self-quenching)

| | |
|--------------------|---|
| Ahl and Cool | JCPSA6-1973-58-5540 |
| Breshears and Bird | JCPSA6-1971-54-2968 |
| Chen, H-L. | JCPSA6-1971-55-5551 |
| Chow and Greene | JCPSA6-1965-43-324 |
| Kapralova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Moore, C. B. | JCPSA6-1965-43-2979 |
| Sentman, L. H. | CHPLBC-1973-18-493 (calc., model.) |
| Shin, H. K. | JPCHAX-1971-75-1079 |

C. $\text{HI}^{\ddagger}(\text{DI}^{\ddagger})$ Theoretical papers

| | |
|-------------------|--|
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| Ben-Shaul, et al. | JCPSA6-1972-57-5427 (calc., pop. distr.) |
| Henry, et al. | CHPLBC-1973-20-138 (r.p., traj.) |
| Kapralova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Moore, C. B. | JCPSA6-1965-43-2979 |
| Sentman, L. H. | CHPLBC-1973-18-493 (calc., model.) |
| Shin, H. K. | JPCHAX-1971-75-1079 |

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| Borrell, P. | BOOKA7-1969-2-180 |
| Carrington and Garvin | CCHKAZ-1969-3-174 |
| Carrington and Polanyi | 26BMAD-1972-9-135 |
| Chester, A. N. | LSRVAN-1971-7-25 |
| Chester and Hess | IEJQA7-1972-8-1 |
| Cohen, N. | XADRCA-1972-AD 763715 |
| Cool, T. A. | BOOKA7-1971-197 |
| Cool, T. A. | IEJQA7-1973-9-72 |
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| Emanuel, et al. | XADRCA-1972-AD 746685 |
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| Kerber, et al. | IEJQA7-1973-9-94 |
| Kompa, K. L. | ACIEAY-1970-9-773 |
| Kompa, K. L. | CITEAH-1970-42-573 |
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| Moore, C. B. | BOOKA7-1967-133 |
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| Rabinovitch and Flowers | QRCSAL-1964-18-122 |
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| U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET | | 1. PUBLICATION OR REPORT NO. NBS SP-392 | 2. Gov't Accession No. | 3. Recipient's Accession No. |
| 4. TITLE AND SUBTITLE Vibrationally Excited Hydrogen Halides: A Bibliography on Chemical Kinetics of Chemiexcitation and Energy Transfer Processes (1958 through 1973) | | | 5. Publication Date April 1974 | |
| | | | 6. Performing Organization Code | |
| 7. AUTHOR(S) Francis Westley | | | 8. Performing Organ. Report No. | |
| 9. PERFORMING ORGANIZATION NAME AND ADDRESS NATIONAL BUREAU OF STANDARDS DEPARTMENT OF COMMERCE WASHINGTON, D.C. 20234 | | | 10. Project/Task/Work Unit No. | |
| | | | 11. Contract/Grant No. AFOSR-ISSA-74-0001-1 | |
| 12. Sponsoring Organization Name and Complete Address (Street, City, State, ZIP) NBS Office of Standard Reference Data, Air Force Office of Scientific Research 1400 Wilson Blvd., Arlington, Va. 22209 | | | 13. Type of Report & Period Covered Interim | |
| | | | 14. Sponsoring Agency Code | |
| 15. SUPPLEMENTARY NOTES Library of Congress Catalog Card No.: 74-5358. | | | | |
| 16. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.) A bibliography, a reaction oriented list of references, is provided for published papers and reports containing rate data for reactions of halogen atoms with hydrogen-containing compounds, or of H (D, or T) atoms with halogen-containing compounds to form vibrationally chemiexcited hydrogen halides. The reactions for vibroexcitation of hydrogen halides through unimolecular or photochemical elimination, as well as the processes for vibrational energy transfer between hydrogen halides and various second bodies are also included. In addition, four lists of theoretical papers and a list of critical reviews and bibliographies are provided. Over 300 papers covering 50 types of reactions are listed. The period covered extends from 1958 through 1973. | | | | |
| 17. KEY WORDS (six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons) Bibliography; chemical kinetics; chemiexcitation; gas phase; halogens; hydrogen; hydrogen halides; laser; quenching; vibrational energy transfer. | | | | |
| 18. AVAILABILITY <input checked="" type="checkbox"/> Unlimited <input type="checkbox"/> For Official Distribution. Do Not Release to NTIS <input type="checkbox"/> Order From Sup. of Doc., U.S. Government Printing Office Washington, D.C. 20402, SD Cat. No. C13-10:392 <input type="checkbox"/> Order From National Technical Information Service (NTIS) Springfield, Virginia 22151 | | 19. SECURITY CLASS (THIS REPORT) UNCLASSIFIED | | 21. NO. OF PAGES 81 |
| | | 20. SECURITY CLASS (THIS PAGE) UNCLASSIFIED | | 22. Price \$1.30 |

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